

The spectrum and the phase transition of models solvable through the full interval method

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Abstract

The most general exclusion single species reaction-diffusion models with nearest-neighbor interactions on a one dimensional lattice are investigated, for which the evolution of full intervals are closed. Using a generating function method, the probability that n consecutive sites be full is investigated. The stationary values of these probabilities, as well as the spectrum of the time translation generator (Hamiltonian) of these are obtained. It is shown that depending on the reaction rates the model could exhibit a dynamical phase transition.

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1 Introduction

Different methods have been used to study non equilibrium statistical models; including analytical and asymptotic methods, mean-field methods, and large-scale numerical methods. Although mean field solutions may be suitable for higher dimensions, in low dimensional cases fluctuation effects may cause mean field results to differ from the real ones. One dimensional models, which are usually easier to investigate, helps us gaining more knowledge on systems far from equilibrium [1–13]. Many techniques are used to obtain exact results in one-dimensional models. The empty interval method (EIM) is one of them. The full interval method (FIM) is another, which is equivalent to EIM. In EIM, the aim is to calculate the probability that n consecutive sites be empty, E_n . In FIM, one studies the probability that n consecutive sites be full, F_n . In [14–17], one dimensional models have been studied in which some of the reaction rates are infinite, so that it is the (finite) diffusion rates which determine the evolution. These models have been through EIM. In [18], a system with three-site interactions has been studied by EIM. In [19], a generalization of EIM has been used to investigate a one dimensional Potts model with q -states, in the zero-temperature limit. In [20], a classification has been given for one dimensional reaction-diffusion models with nearest neighbor interactions, which are solvable through EIM, by which it is meant that the evolution equations for E_n 's are closed. In such systems, the time derivative of the empty intervals is linear in the empty intervals (and contains no other dynamical variable). If some extra conditions are met (there is no reaction which produces particles in two adjacent sites) the evolution equation for E_n becomes n -independent. This makes solving the evolution equations easier. In [21–23], these were generalized to systems with multi-species systems and multi-site interactions. In [24], the extra condition that the evolution equations for E_n be n -independent was relaxed, and solvable (in the sense of EIM) models on continuum were studied.

In [25], a generalization of EIM was introduced, by which a model was investigated which was not solvable through conventional EIM. In [26, 27], EIM has been used to study the coagulation-diffusion process on a one dimensional chain.

In a recent article, the most general exclusion single species one dimensional reaction-diffusion models with nearest-neighbor interactions were studied, which are both autonomous and can be solved exactly through the full interval method [28]. There, using a generating function method, the general solution for F_n , the probability that n consecutive sites be full, and some other correlation functions of number operators were explicitly obtained.

In this article we relax the condition of autonomy, and study the most general exclusion single species reaction-diffusion models with nearest-neighbor interactions on a one dimensional lattice, which can be solved exactly through full interval method. The change of empty interval to full interval is, of course, not important, as a simple interchange of particles and holes would do that. The scheme of the paper is as follows. In Section 2, the most general exclusion single species one dimensional reaction-diffusion models with nearest-neighbor inter-

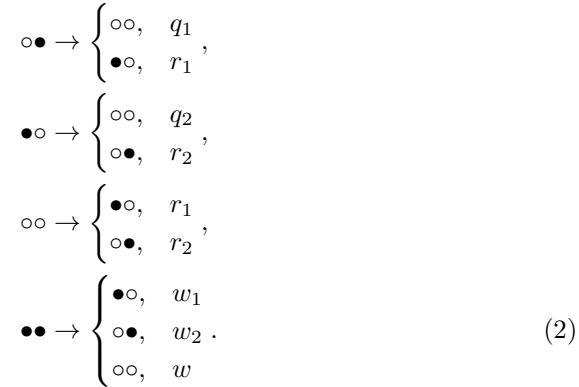
actions are introduced, which can be solved exactly through FIM. In Section 3, a generating function method is used to obtain the time independent solutions to the evolution of full intervals. In Section 4, a similar generating function method is used to study the spectrum of the time translation generator (Hamiltonian) of the full intervals. It is shown that the model may exhibit a dynamical phase transition.

2 Full interval equation

Consider a one dimensional lattice, any site of which is either occupied by a single particle or empty. The full interval F_n is defined as the probability that n consecutive sites be full

$$F_n := P(\overbrace{\bullet \bullet \dots \bullet}^n). \quad (1)$$

An empty (occupied) site is denoted by \circ (\bullet). Assuming only nearest neighbor interactions, it can be seen ([24]) that the necessary and sufficient condition that the evolution equations for F_n 's be closed is that only the following reactions be present, and their rates be related to each other as follows.



The equality of some rates, means that the rates of the reactions $(\circ\circ \rightarrow \bullet\circ)$ and $(\circ\bullet \rightarrow \bullet\circ)$ are the same, and the rates of the reactions $(\circ\circ \rightarrow \circ\bullet)$ and $(\bullet\circ \rightarrow \circ\bullet)$ are the same as well.

As in, for example [24], it can be seen that the time evolution equation for F_n is

$$\begin{aligned} \frac{dF_n}{dt} &= (r_1 + r_2)(F_{n-1} + F_{n+1} - 2F_n) - (q_1 + q_2)(F_n - F_{n+1}) \\ &\quad - (n-1)(w_1 + w_2 + w)F_n - (w_1 + w_2 + 2w)F_{n+1}, \quad n \geq 2 \\ \frac{dF_1}{dt} &= (r_1 + r_2)(1 + F_2 - 2F_1) - (q_1 + q_2)(F_1 - F_2) \\ &\quad - (w_1 + w_2 + 2w)F_2. \end{aligned} \quad (3)$$

It is seen that defining

$$F_0 := 1, \quad (4)$$

the evolution equation for F_1 takes a form similar to that of other F_n 's:

$$\begin{aligned} \frac{dF_n}{dt} = & (r_1 + r_2)(F_{n-1} + F_{n+1} - 2F_n) - (q_1 + q_2)(F_n - F_{n+1}) \\ & - (n-1)(w_1 + w_2 + w)F_n - (w_1 + w_2 + 2w)F_{n+1}, \quad n \geq 1. \end{aligned} \quad (5)$$

Comparing this with the similar expression in, it is seen that in [24] there is no term analogues to the last term here. In [28], it is assumed the models to be autonomous, which leads to removing the term F_{n+1} from (5).

Defining

$$\tilde{t} := (w_1 + w_2 + w)t, \quad (6)$$

one arrives at

$$\frac{dF_n}{d\tilde{t}} = bF_{n-1} - (a + n - 1)F_n + cF_{n+1}, \quad (7)$$

where

$$\begin{aligned} a &:= \frac{2(r_1 + r_2) + q_1 + q_2}{w + w_1 + w_2}, \\ b &:= \frac{r_1 + r_2}{w + w_1 + w_2}, \\ c &:= \frac{r_1 + r_2 + q_1 + q_2 - 2w - w_1 - w_2}{w + w_1 + w_2}. \end{aligned} \quad (8)$$

The case $(w_1 + w_2 + w) = 0$, will be dealt with separately. For simplicity, hereafter the symbol t is used in place of \tilde{t} , so

$$\frac{dF_n}{dt} = bF_{n-1} - (a + n - 1)F_n + cF_{n+1}. \quad (9)$$

A generating function F is also defined, which will be used later:

$$F(x) := \sum_{n=0}^{\infty} \frac{F_n x^n}{n!}. \quad (10)$$

It is seen that

$$F_n = F^{(n)}(0), \quad (11)$$

where $F^{(n)}$ is the n -th derivative of F .

3 The time independent equation

The time independent solution F^{st} satisfies

$$bF_{n-1}^{\text{st}} - (a + n - 1)F_n^{\text{st}} + cF_{n+1}^{\text{st}} = 0, \quad (12)$$

which yields

$$\sum_{n=1}^{\infty} \frac{x^{n-1}}{(n-1)!} [cF_{n+1}^{\text{st}} + bF_{n-1}^{\text{st}} - (a + n - 1)F_n^{\text{st}}] = 0, \quad (13)$$

so that

$$(c-x) \frac{d^2 F^{\text{st}}}{dx^2} - a \frac{dF^{\text{st}}}{dx} + b F^{\text{st}} = 0. \quad (14)$$

Defining

$$\begin{aligned} F^{\text{st}}(x) &:= z^{(1-a)} G^{\text{st}}(z), \\ z &:= 2 \sqrt{b(c-x)}, \end{aligned} \quad (15)$$

one arrives at

$$z^2 \frac{d^2 G^{\text{st}}}{dz^2} + z \frac{dG^{\text{st}}}{dz} + [z^2 - (1-a)^2] G^{\text{st}} = 0. \quad (16)$$

So,

$$G^{\text{st}}(z) = \alpha J_{a-1}(z) + \beta J_{1-a}(z), \quad (17)$$

where J_ν is the Bessel function of order ν , and α and β are constants. So,

$$\begin{aligned} F^{\text{st}}(x) &= \alpha [2\sqrt{b(c-x)}]^{(1-a)} J_{a-1}[2\sqrt{b(c-x)}] \\ &\quad + \beta [2\sqrt{b(c-x)}]^{(1-a)} J_{1-a}[2\sqrt{b(c-x)}]. \end{aligned} \quad (18)$$

As F_n^{st} is in $[0, 1]$, the convergence radius of the series defining F^{st} is infinity. So the generating function F^{st} as a function of x is analytic on the entire complex plane. Using

$$J_\nu(z) = \frac{1}{\Gamma(\nu+1)} \left(\frac{z}{2}\right)^\nu + \dots, \quad |z| \ll 1, \quad (19)$$

the analyticity of F^{st} at $(x=c)$ demands that

$$\beta = 0. \quad (20)$$

As

$$F_0^{\text{st}} = 1, \quad (21)$$

one has

$$F^{\text{st}}(0) = 1, \quad (22)$$

which can be exploited to obtain α . So,

$$F^{\text{st}}(x) = \frac{[2\sqrt{b(c-x)}]^{(1-a)} J_{a-1}[2\sqrt{b(c-x)}]}{(2\sqrt{bc})^{(1-a)} J_{a-1}(2\sqrt{bc})}. \quad (23)$$

Using (11), one can find F_n . One has

$$\begin{aligned} \left(\frac{d}{dx}\right)^n F^{\text{st}}(x) &= \frac{1}{(2\sqrt{bc})^{1-a} J_{a-1}(2\sqrt{bc})} \left(-\frac{2b}{z} \frac{d}{dz}\right)^n [z^{1-a} J_{a-1}(z)], \\ &= \frac{1}{(2\sqrt{bc})^{1-a} J_{a-1}(2\sqrt{bc})} (2b)^n z^{1-a-n} J_{a-1+n}(z), \end{aligned} \quad (24)$$

which results in

$$F_n^{\text{st}} = \left(\frac{b}{c}\right)^{n/2} \frac{J_{a-1+n}(2\sqrt{bc})}{J_{a-1}(2\sqrt{bc})}. \quad (25)$$

There are two limiting cases to be studied separately:

i: $b = 0$.

This can be studied as the limit $b \rightarrow 0$ of the general case. Using (25) and the limiting behavior (19), one arrives at

$$F_n^{\text{st}} = \frac{\Gamma(a)}{\Gamma(a+n)} b^n, \quad b \ll 1, \quad (26)$$

which leads to

$$\lim_{b \rightarrow 0} F_n^{\text{st}} = \delta_n^0. \quad (27)$$

This is the case if a is nonzero. If a and b both vanish, the result could be obtained directly from (12) to be

$$F_n^{\text{st}} = \begin{cases} \rho, & n = 1 \\ 0, & n > 1 \end{cases}, \quad (28)$$

where

$$0 \leq \rho \leq \frac{1}{2}, \quad (29)$$

and it has been assumed that at least one of the rates are nonvanishing. One notes that ρ is in fact the density of the particles, and the restriction on its value results from the fact that in the stationary configuration no two-adjacent sites are full.

These results are expected. If b vanishes but a does not, there are no reactions which produce particles but there are reactions which annihilate particles, whether the particles are adjacent to holes or other particles. So at large time the lattice becomes empty. If both a and b vanish, there are no reactions which produce particles, but there are reactions which annihilate particles, only if there are two neighboring particles. So particles will be annihilated, but when there are particles with empty neighboring sites, they will survive.

In fact, regarding the stationary solution as the large-time solution, one can obtain an expression for ρ in terms of the initial conditions. As both a and b vanish, one has

$$\frac{dF_n}{dt} = -(n-1)F_n + cF_{n+1}. \quad (30)$$

Defining

$$\mathcal{F}_n(t) := \exp[(n-1)t] F_n(t), \quad (31)$$

equation (30) is recast to

$$\frac{d\mathcal{F}_n}{dt} = c \exp(-t) \mathcal{F}_{n+1}, \quad (32)$$

which results is

$$\mathcal{F}_n(t) = \sum_{k=0}^{\infty} \frac{[c - c \exp(-t)]^k}{k!} \mathcal{F}_{n+k}(0), \quad (33)$$

so that

$$F_n(t) = \exp[-(n-1)t] \sum_{k=0}^{\infty} \frac{[c - c \exp(-t)]^k}{k!} F_{n+k}(0), \quad (34)$$

from which,

$$F_1(\infty) = \sum_{k=0}^{\infty} \frac{c^k}{k!} F_{1+k}(0), \quad (35)$$

or,

$$\rho = \sum_{k=0}^{\infty} \frac{c^k}{k!} F_{1+k}(0). \quad (36)$$

One notes that when a and b both vanish, c is nonpositive.

ii: $w_1 + w_2 + w = 0$.

In this case all of the rates w_1 , w_2 , and w should vanish. One arrives at

$$\begin{aligned} (r_1 + r_2) F_{n-1}^{\text{st}} - (2r_1 + 2r_2 + q_1 + q_2) F_n^{\text{st}} + (r_1 + r_2 + q_1 + q_2) F_{n+1}^{\text{st}} &= 0, \\ F_0^{\text{st}} &= 1. \end{aligned} \quad (37)$$

The solution to (37) is

$$F_n^{\text{st}} = \zeta + (1 - \zeta) \left(\frac{r_1 + r_2}{r_1 + r_2 + q_1 + q_2} \right)^n, \quad (38)$$

where

$$0 \leq \zeta \leq 1, \quad (39)$$

provided of q_1 and q_2 , at least one is nonvanishing. Otherwise

$$F_n^{\text{st}} = 1, \quad (40)$$

which corresponds to a full lattice.

4 Relaxation towards the time independent equation

To study the spectrum of the time translation generator (Hamiltonian) of the full intervals, again the generating function is used. Defining

$$F_n^{\text{dy}} := F_n - F_n^{\text{st}}, \quad (41)$$

one arrives at

$$\frac{dF_n^{\text{dy}}}{dt} = b F_{n-1}^{\text{dy}} - (a + n - 1) F_n^{\text{dy}} + c F_{n+1}^{\text{dy}}, \quad (42)$$

with the boundary condition

$$F_0^{\text{dy}} = 0. \quad (43)$$

Equation (42) is of the form

$$\frac{dF_n^{\text{dy}}}{dt} = (h F^{\text{dy}})_n, \quad (44)$$

where h is a linear operator. To find this relaxation time, one should obtain the eigenvalues of h . The eigenvalue with the largest real part, determines the relaxation time. Denoting the eigenvector of h corresponding to the eigenvalue E by ψ_E , one has

$$E \psi_{E n} = b \psi_{E n-1} - (a + n - 1) \psi_{E n} + c \psi_{E n+1}, \quad (45)$$

where E is the corresponding eigenvalue. This is similar to (12), with a replaced by $(a + E)$. So repeating similar arguments, one arrives at

$$\psi_E(x) = \alpha (c - x)^{(1-a-E)/2} J_{a+E-1}[2\sqrt{b(c-x)}]. \quad (46)$$

But now the boundary condition is

$$\psi_E(0) = 0, \quad (47)$$

which results in

$$J_{a+E-1}(2\sqrt{bc}) = 0. \quad (48)$$

This gives the spectrum of h .

In the case $b = 0$, one can find more explicit forms for the eigenvalues and eigenvectors. Starting from (45), one arrives at

$$\psi_{E n+1} = \frac{E + a + n - 1}{c} \psi_{E n}. \quad (49)$$

This recursive relations shows that $\psi_{E n}$ tends to infinity as n tends to infinity, unless there is a k so that $\psi_{E n}$'s vanish for $n > k$. This happens if E is equal to one of E_k 's, where

$$E_k = 1 - a - k, \quad (50)$$

and k is a positive integer. Denoting the corresponding eigenvector by ψ_k instead of ψ_E , one would arrive at

$$\psi_{k n} = \frac{(-c)^{k-n}}{\Gamma(k+1-n)} \psi_{k k}. \quad (51)$$

The relaxation time of the system is obtained from the largest real part of the eigenvalues, which in this case is $(-a)$. So

$$\tau = \frac{1}{a}, \quad (bc) = 0. \quad (52)$$

Defining

$$\varepsilon := E + a - 1, \quad (53)$$

it is seen from (48) that ε depends on only the product (bc) . So the expression (50) holds for the case $c = 0$ as well. The case $c = 0$ has already been discussed in greater detail in [28]

From (8) it is seen that b is nonnegative, while c can change sign. These expressions also show that

$$-1 \leq (bc), \quad (54)$$

but there is no upper limit for (bc) .

For (bc) near zero, one can find the leading correction to (51) as follows. Defining

$$\delta_k := \varepsilon_k + k, \quad (55)$$

equation (48) becomes

$$J_{-k+\delta_k}(2\sqrt{bc}) = 0, \quad (56)$$

which is, up to the leading order, equivalent to

$$1 - \frac{(bc)^k}{k!(k-1)!\delta_k} = 0, \quad (57)$$

showing that

$$\delta_k = \frac{(bc)^k}{k!(k-1)!} + \dots, \quad |bc| \ll k^2. \quad (58)$$

So one has,

$$\tau = \frac{1}{a - bc} + \dots, \quad |bc| \ll 1. \quad (59)$$

If (bc) is positive, there is an inner product with respect to which h is Hermitian. So if (bc) is positive, the spectrum of h is real. Increasing (bc) from zero, the values of ε_k 's are also increased. For large values of (bc) one can find the values of ε_k 's using various asymptotic expressions of the Bessel functions. One arrives at

$$\varepsilon_k = \begin{cases} 2\sqrt{bc} - \mathfrak{a}_k (bc)^{1/6} + \dots, & k \ll (bc)^{1/3} \\ \frac{4\sqrt{bc}}{\pi} + \frac{3}{2} - 2k + \dots, & |\varepsilon_k| \ll (bc)^{1/2}, \\ -k + \frac{(bc)^k}{k!(k-1)!} + \dots, & k \gg (bc)^{1/2} \end{cases} \quad (60)$$

where $(-\mathfrak{a}_k)$ is the k 'th zero of the Airy function. The largest of ε_k 's determine the relaxation time. One then has

$$\tau = \frac{1}{a - 1 + 2\sqrt{bc}} + \dots, \quad (bc) \gg 1. \quad (61)$$

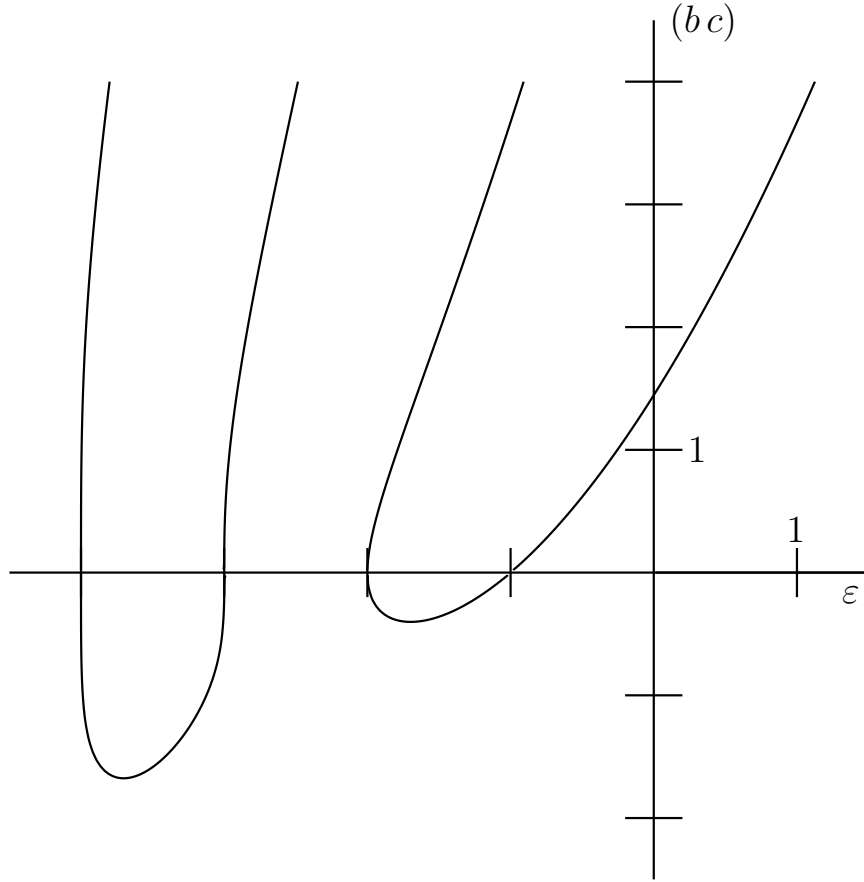


Figure 1:
The plot of (bc) versus ε , corresponding to the four largest eigenvalues of h

From (8) it is seen that for nonnegative c ,

$$(a - 1) \geq 2\sqrt{bc}. \quad (62)$$

For a negative (bc) , however, there are cases where the spectrum of h is not real. A plot of (bc) in terms of (real) ε for

$$J_\varepsilon(2\sqrt{bc}) = 0, \quad (63)$$

shows that there is one minimum for (bc) for each interval $\varepsilon \in (-2n, -2n+1)$, where n is a positive integer, figure 1. However, only the minimum corresponding to $\varepsilon \in (-2, -1)$ is larger than (-1) . So there is a critical value for (bc) , at which two of the eigenvalues of h (the largest and the next largest) become

equal, and if (bc) is less than that critical value, two of the eigenvalues of h become nonreal (complex conjugates of each other). Denoting that critical value of (bc) by γ , and the corresponding value of ε by ε_{tr} , one arrives at the following approximate expression for ε and (bc) near their critical value.

$$(bc) = \gamma + \frac{(\varepsilon - \varepsilon_c)^2}{\nu}, \quad (64)$$

where the numerical values of the constants in the above equation are

$$\begin{aligned} \gamma &= -0.401873, \\ \nu &= 0.754464, \\ \varepsilon_c &= -1.697524. \end{aligned} \quad (65)$$

One then arrives at the following expression for ε_1 , for (bc) near the critical value γ :

$$\varepsilon_1 = \varepsilon_c + \sqrt{\nu(bc - \gamma)}, \quad (66)$$

resulting to

$$\tau = \begin{cases} \frac{1}{a - 1 - \varepsilon_c - \sqrt{\nu(bc - \gamma)}}, & (bc) \gtrsim \gamma \\ \frac{1}{a - 1 - \varepsilon_c}, & (bc) \lesssim \gamma \end{cases}. \quad (67)$$

So the derivative of the relaxation time with respect to (bc) , is infinite for $(bc) \rightarrow \gamma^+$, and zero for $(bc) \rightarrow \gamma^-$. This model shows a dynamical phase transition.

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